

2,2,8-Trimethyl-7-prop-2-ynoxychromene
94244-29-8 | DTXSID10241225

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.59

Global applicability domain: Inside

Local applicability domain index: 6.14e-01

Confidence level: 6.69e-01

Nearest Neighbors from the Training Set

Image not found

MCPB ethyl

Measured: 4.26

Predicted: 3.27